Dynamical Solutions to the Ground State of a Frustrated Magnet*

Author: Scott Salmon
Supervisor: Dr. David Feder
University of Calgary - Faculty of Science - Department of Physics and Astronomy

Frustrated magnets are challenging to model due to their degenerate ground states, stemming from competing lattice interactions. Their vast configuration space and complex interactions make classical computational methods inadequate. This project aims to develop a novel simulation approach for frustrated magnets, inspired by the Gross-Pitaevskii equation,[1] by incorporating non-linearity at lattice boundaries via a mean-field approximation to better approximate ground states. The ultimate goal is to establish a scalable framework that can be extended to quantum computing platforms for studying larger systems. [2]

The work completed this semester has focused on building the foundational components of a program to simulate a frustrated magnet system. Once these components are finalized, the next phase will involve integrating non-linearity into the model, aligning with our broader objective. The first step in simulating frustration was achieved by introducing geometric frustration via the construction of a triangular lattice. This triangular structure was generated from a conventional $N \times M$ lattice, which typically forms a square configuration, as shown on the left in Figure 1. However, due to the specific interactions defined between neighboring sites, the effective lattice takes on a triangular form, as illustrated on the right in Figure 1.

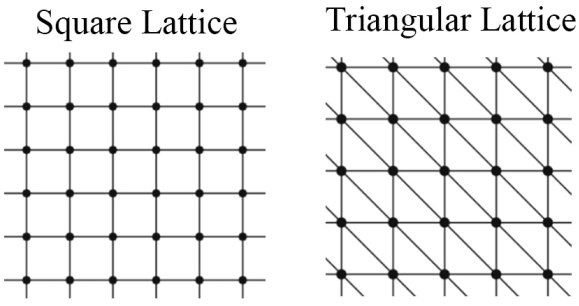

Figure 1: Diagram showing how a triangular lattice is created using a $N \times M$ grid. [3]

Each site's spin is represented by +1 (spin up) or -1 (spin down). To calculate the total energy of the system, I developed a function based on a Hamiltonian that accounts for pairwise spin interactions, the Ising Model (simplified): [4]

$$H(\sigma) = -J \sum_{i,j} \sigma_i \sigma_j$$

where H represents the total energy of a given configuration, J is the coupling constant, and σ_i and σ_j are the spin states of neighboring sites. To construct the triangular lattice, the program considers neighbors directly to the right, directly below, and diagonally to the lower right. Additionally, periodic boundary conditions are applied to simulate an infinite lattice, ensuring that interactions extend beyond the edges of the lattice.

With a method to calculate the energy of a given configuration established, the next step is to generate all possible configurations in order to identify those with the lowest energy. To accomplish this, I implemented a function that converts bit strings into spin states, where "1"s correspond to up spins and "0"s correspond to down spins.

For example, consider a rectangular lattice with dimensions $N = 3$ and $M = 5$. The total number of possible configurations on the grid is $(2^{N \times M} - 1)$, or 32 767. In bitwise notation, configuration 0 is represented as 00000 00000 00000, configuration 1 as 00000 00000 00001, configuration 2 as 00000 00000 00010 and so on, up to configuration 32,767 as 11111 11111 11111.

This representation enables us to iterate through all possible configurations for a given $N \times M$ grid size, and it allows us to efficiently store any desired configuration(s) as bit strings that can easily be referenced later.

As the function iterates through all possible configurations, the Hamiltonian function is applied to determine the energy of each configuration. I

then implemented a check to compare the energy of the current configuration with the energies from previous iterations. If the current configuration's energy is lower, the corresponding bit string is stored. If the current configuration's energy is equal to the previous low, then the current configuration is added to the list of lowest configurations. This step is crucial, as we know that at the ground state, the system will be in a superposition of all the lowest-energy configurations.

Now that we have identified all of the lowest-energy configurations, the next step is to determine the correlated spin states for each dipole. This is important because it allows us to identify which dipoles in the lattice are stable (i.e., not frustrated) when the system reaches its lowest energy state, and which dipoles are constantly changing (i.e., frustrated). We will determine the correlated spin states using the Pauli matrices, specifically the Pauli matrix in the z-direction:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Using this matrix, along with the quantum state of the system (represented as $|\psi\rangle$), we can find the spin correlations between each dipole through the following tensor formula:

$$C_{ij} = \langle \psi | \sigma_z \otimes \sigma_z | \psi \rangle$$

By calculating the spin correlations between neighboring dipoles using Pauli matrices, we can assess the degree of correlation between spins. This will help us understand how frustration manifests in the system, with highly correlated spins indicating stability and weak or no correlations suggesting frustration in the system's ground state.

Throughout the next semester, the first step will be to integrate the correlated spin states into the program that has been developed thus far. Once this is accomplished, we will be able to pinpoint which specific dipoles are frustrated in the system, effectively simulating a frustrated magnet. With this foundation in place, we can then move forward with incorporating non-linearity into the system, which will align with our broader objective of approximating the true ground state more accurately.

Overall, I will continue refining the simulation by integrating the correlated spin states and addressing the challenges of accurately modeling frustration within the system. Additionally, I will focus on optimizing the computational efficiency, ensuring that the program can handle larger lattice sizes and more complex configurations. Once the foundational components are fully implemented, I plan to incorporate non-linearity using a mean-field approximation, further advancing our ability to approximate the true ground state. This will ultimately prepare the system for potential implementation on quantum computing platforms, enabling us to explore larger and more intricate frustrated magnet systems.

[∗] Physical Review A (PRA) Journal Style

[1] L. Pitaevskii and S. Stringari, *Bose-Einstein Condensation* (Clarendon Press, 2003).
[2] J. Zhang, M. Yung, R. Laflamme, A. Aspuru-Guzik, and J. Baugh, Nature Communications **3** (2012).
[3] M. Kotani and T. Sunada, Mathematische Zeitschrift **254**, 837 (2006).
[4] A. Shekaari and M. Jafari, *Theory and simulation of the ising model* (2021).